Structural Methods in Inorganic Chemistry
CHEM 475/CHEM 575
Syllabus
Spring 2022

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Text: *Structural Methods in Molecular Inorganic Chemistry,* D. W. H. Rankin, Norbert Mitzel, Carole Morrison*,* ISBN: 978-0-470-97278-6

Structural Methods in Inorganic Chemistry is a survey course of selected advanced techniques for characterizing inorganic and organometallic compounds. The methods covered are listed below.

Unit 1

Group Theory
Vibrational Spectroscopy
Electronic Spectroscopy

Unit 2

Nuclear Magnetic Resonance Spectroscopy
Electron Paramagnetic Resonance Spectroscopy
Mössbauer Spectroscopy
Mass Spectrometry

Unit 3

X-ray Diffraction

Tentative Exam Schedule	
Unit 1	February 3, 2022
Unit 2	March 10, 2022
Unit 3	April 12, 2022

The course grade for **CHEM 475** will be determined from class participation (10%), three in-class exams (25% each) and an oral in-class presentation (15%).

For **CHEM 575**, the course grade will be determined from class participation (10%), three exams (20% each), an oral in-class presentation (15%) and literature reports (15%).

Rubrics for the in-class presentations and the literature reports will be provided. The literature reports, which are required only for students enrolled in CHEM 575, will be due on February 8, March 22 and April 19.

Accommodations of Disabilities

If you have a documented disability that is registered with Disability Resource Center (adarice@rice.edu, Allen Center, Room 111), please provide Professor Whitmire or Professor Marti with documentation from the DRC indicating what the accommodations should be for the class. This information should be provided before the end of the second week of classes.

Learning Outcomes

This course will teach advanced structural characterization methods for inorganic and organometallic molecules. Students should develop understanding in the following topics:

- Identification of molecular symmetry elements and the assignment of molecules to point groups
- Group theory and the selection rules for vibrational spectroscopy (infrared and Raman spectroscopy) and electronic spectroscopy
- Understanding how vibrational spectra are affected by molecular symmetry.
- The selection rules for electronic spectroscopy and the information this technique provides for electronic configurations of transition metal complexes.
- Understanding nuclear magnetic resonance spectroscopy beyond the fundamental ^{1}H and ^{13}C NMR spectroscopies covered in introductory organic chemistry classes. This will include NMR of other nuclei found in inorganic molecules including ^{19}F, ^{31}P and a variety of transition metals that are spin 1/2 nuclei, as well as coupling patterns exhibited when multiple NMR active nuclei are present in the same molecule. Dynamic processes of molecules in solution will be examined by variable temperature NMR.
- Interpretation of Electron Paramagnetic Resonance spectra (also known as Electron Spin Resonance) to determine the presence and location of unpaired electrons in molecules
- Mössbauer Spectroscopy and what information it provides about the symmetry of certain metal coordination environments
- Mass spectrometry and how to identify complex molecules from isotope distribution and fragmentation patterns
- Identification of solid state symmetry elements and the assigning of solids to space groups
- Collection, solution and refinement of single crystal X-ray diffraction data to give solid state structures. This will include an introduction to understanding common crystallographic data presented in publications such as unit cell parameters, space groups and symmetry, crystallographic vs. molecular symmetry, Z values, residuals, etc.